

<http://www.cas.org/support/stngen/stdoc/properties.html>

=> s ibuprofen/cn

L1 1 IBUPROFEN/CN

=> d

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN

RN 15687-27-1 REGISTRY

ED Entered STN: 16 Nov 1984

CN Benzeneacetic acid, α -methyl-4-(2-methylpropyl)- (CA INDEX NAME)

OTHER NAMES:

CN (\pm)- α -Methyl-4-(2-methylpropyl)benzeneacetic acid

CN (\pm)-2-(p-Isobutylphenyl)propionic acid

CN (\pm)-Ibuprofen

CN (\pm)-Ibuprophen

CN (4-Isobutylphenyl)- α -methylacetic acid

CN (RS)-Ibuprofen

CN α -(4-Isobutylphenyl)propionic acid

CN α -Methyl-4-(2-methylpropyl)benzeneacetic acid

CN 2-(4'-Isobutylphenyl)propionic acid

CN 2-(4-Isobutylphenyl)propanoic acid

CN 2-(p-Isobutylphenyl)propionic acid

CN 4-Isobutyl- α -methylphenylacetic acid

CN 4-Isobutylhydratropic acid

CN Act 3

CN Actiprofen

CN Adex 200

CN Adran

CN Advil

CN Alaxan

CN Algi-Flanderil

CN Algiflex

CN Algofen

CN Am-Fam 400

CN Amibufen

CN Anafen

CN Anco

CN Andran

CN Anflagen

CN Antarene

CN Antiflam

CN Apo-Ibuprofen

CN Apsifen

CN Artofen

CN Artril

CN Artril 300

CN Atril 300

CN Balkaprofen

CN Betaprofen

CN Bloom

CN Bluton

CN Brofen

CN Brufanic

CN Brufen

10/923,271

CN Brufen 400
CN Brufen Retard
CN Bruflam
CN Brufort
CN Buburone
CN Buluofen
CN Burana
CN Ibuprofen

ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT - Use FCN, FIDE, or ALL for DISPLAY

DR 58560-75-1, 139466-08-3

MF C13 H18 O2

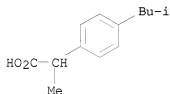
CI COM

LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CABA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCAIS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DRUGU, EMBASE, HSDB*, IFICDB, IFIPAT, IFIUDB, IMSCOSEARCH, IMSDRUGNEWS, IMSPATENTS, IMSPRODUCT, IMSRESEARCH, IPA, MEDLINE, MRCK*, MSDS-OHS, PATDPASPC, PHAR, PIRA, PROMT, PROUSDDR, PS, RTECS*, SCISEARCH, SPECINFO, SYNTHLINE, TOXCENTER, ULIDAT, USAN, USPAT2, USPATFULL, USPATOLD, VETU

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**, WHO

(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10189 REFERENCES IN FILE CA (1907 TO DATE)

295 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

10234 REFERENCES IN FILE CAPLUS (1907 TO DATE)

2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

7.61

8.30

FILE 'CAPLUS' ENTERED AT 16:22:15 ON 17 APR 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available

for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 17 Apr 2008 VOL 148 ISS 16

FILE LAST UPDATED: 16 Apr 2008 (20080416/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

```
=> s 15687-27-1/prep
      10234 15687-27-1
      4559046 PREP/RL
L2      664 15687-27-1/PREP
      (15687-27-1 (L) PREP/RL)

=> s 15687-27-1/proc
      10234 15687-27-1
      4312272 PROC/RL
L3      1261 15687-27-1/PROC
      (15687-27-1 (L) PROC/RL)

=> s 15687-27-1/pur
      10234 15687-27-1
      278306 PUR/RL
L4      59 15687-27-1/PUR
      (15687-27-1 (L) PUR/RL)

=> s 12 or 13 or 14
L5      1904 L2 OR L3 OR L4

=> s 15 and palladium
      176569 PALLADIUM
L6      70 L5 AND PALLADIUM

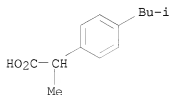
=> s 16 and py<2003
      22929815 PY<2003
L7      52 L6 AND PY<2003

=> s 17 and (activated carbon or silica gel or aluminum oxide or adsor? or ion
exchange resin or zeolite)
      555617 ACTIVATED
      1356558 CARBON
      53030 ACTIVATED CARBON
      (ACTIVATED(W)CARBON)
      569020 SILICA
      534872 GEL
      96261 SILICA GEL
      (SILICA(W)GEL)
      1030281 ALUMINUM
```

1856565 OXIDE
 102924 ALUMINUM OXIDE
 (ALUMINUM(W)OXIDE)
 632611 ADSOR?
 1253908 ION
 602580 EXCHANGE
 662782 RESIN
 18493 ION EXCHANGE RESIN
 (ION(W)EXCHANGE(W)RESIN)
 106213 ZEOLITE
 L8 4 L7 AND (ACTIVATED CARBON OR SILICA GEL OR ALUMINUM OXIDE OR ADSO
 R? OR ION EXCHANGE RESIN OR ZEOLITE)

=> d 1-4 ibib abs hitstr

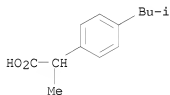
L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2002:552598 CAPLUS
 DOCUMENT NUMBER: 137:249479
 TITLE: Anchored Pd Complex in MCM-41 and MCM-48: Novel
 Heterogeneous Catalysts for Hydrocarboxylation of Aryl
 Olefins and Alcohols
 AUTHOR(S): Mukhopadhyay, Kausik; Sarkar, Bibhas R.; Chaudhari,
 Raghunath V.
 CORPORATE SOURCE: Homogeneous Catalysis Division, National Chemical
 Laboratory, Pune, 411008, India
 SOURCE: Journal of the American Chemical Society (2002
), 124(33), 9692-9693
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Synthesis of anchored Pd complexes in mesoporous supports such as MCM-41
 and MCM-48 as true heterogeneous catalysts for hydrocarboxylation of aryl
 olefins and alcs. to give excellent conversion (.apprx.100%) and
 regioselectivity (.apprx.99%) for 2-arylpropionic acids. The catalysts
 were characterized by powder-XRD, 31P CP-MAS NMR, FT-IR, TEM, XPS and
 ICP-AES. Recycle studies with these anchored Pd mesoporous catalysts were
 performed to confirm true heterogeneity.
 IT 15687-27-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (hydrocarboxylation of aryl olefins and alcs. catalyzed by anchored Pd
 complexes in mesoporous supports such as MCM-41 and MCM-48)
 RN 15687-27-1 CAPLUS
 CN Benzeneacetic acid, α -methyl-4-(2-methylpropyl)- (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1998:228466 CAPLUS
 DOCUMENT NUMBER: 128:309668
 TITLE: Catalytic carbonylation for the synthesis of chemical intermediates
 AUTHOR(S): Kim, Young Gul; Lee, Jae Sung; Lee, Kyung Hee
 CORPORATE SOURCE: Department of Chemical Engineering and School of Environmental Engineering, Pohang Univ. of Science and Technology, Pohang, 790-784, S. Korea
 SOURCE: Research on Chemical Intermediates (1998), 24(2), 197-211
 CODEN: RCINEE; ISSN: 0922-6168
 PUBLISHER: VSP BV
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Chemical related to three catalytic carbonylation reactions is discussed. Synthesis of diphenylurea from nitrobenzene, aniline, and CO gives isolated yields above 98% at 100°-120° and 15-60 bar of CO in the presence of a palladium(II) complex, PPh3 and Net4Cl . Exptl. evidence was provided to prove a new reaction stoichiometry and involvement of a carbamoyl intermediate. In carbonylation of HCHO over ion exchange resin catalysts, reaction temperature, time, pressure, and solvent were important variables to obtain high yields of Me glycolate. Carbonylation of isobutylphenylethanol at 120° and 40 bar of CO in the presence of $\text{PdCl}_2\text{-PPh}_3\text{-HCl}$ gives 98% yield of α -(4-isobutylphenyl) propionic acid (ibuprofen). Each catalyst component had a definite role that is indispensable for an efficient overall reaction.
 IT 15687-27-1P, α -(4-Isobutylphenyl)propionic acid
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (catalytic hydrocarbonylation for synthesis of isobutylphenyl propionic acid)
 RN 15687-27-1 CAPLUS
 CN Benzeneacetic acid, α -methyl-4-(2-methylpropyl)- (CA INDEX NAME)

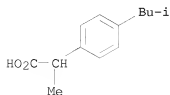


REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1991:228540 CAPLUS
 DOCUMENT NUMBER: 114:228540
 TITLE: Preparation of alpha-(4-isobutylphenyl)propionic acid and its precursors alpha-(4-isobutylphenyl)propionaldehyde and methyl

INVENTOR(S): alpha-(4-isobutylphenyl)propionate from
isobutylbenzene
Tokumoto, Yuuichi; Shimizu, Isao; Inoue, Satoru
PATENT ASSIGNEE(S): Nippon Petrochemicals Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 39 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 414207	A2	19910227	EP 1990-115995	19900821 <--
EP 414207	A3	19911023		
EP 414207	B1	19940803		
R: CH, DE, FR, GB, IT, LI, SE				
JP 03083948	A	19910409	JP 1989-220009	19890825 <--
CA 2023679	A1	19910226	CA 1990-2023679	19900821 <--
CA 2023679	C	19980818		
US 5166419	A	19921124	US 1990-571178	19900822 <--
KR 187301	B1	19990515	KR 1990-13301	19900825 <--
JP 10182541	A	19980707	JP 1998-12856	19980126 <--
JP 2851276	B2	19990127		
PRIORITY APPLN. INFO.:		JP 1989-220009	A	19890825
OTHER SOURCE(S):		CASREACT 114:228540; MARPAT 114:228540		
<p>AB A method for preparing α-(4-isobutylphenyl)propionic acid (I) or its precursors Me α-(4-isobutylphenyl)propionate (II) or α-(4-isobutylphenyl)propionaldehyde (III) at low cost and high purity is claimed. I is a useful medicine (Code name ibuprofen). The method for the preparation of I-III comprises 3 steps: a) subjecting isobutylbenzene and a polyalkylbenzene to disproportionation reaction to form p-isobutyl(ethyl)benzene b) dehydrogenating p-isobutylethylbenzene to form p-isobutylstyrene and c) hydrocarboxylation, hydroesterification, or hydroformylation of p-isobutylstyrene to give I-III resp. Thus, disproportionation reaction of isobutylbenzenes with diethylbenzene in the presence of HY zeolite catalyst gave p-isobutylethylbenzene (64.1 weight % conversion and 46.3 mol % selectivity). Dehydrogenation of p-isobutylethylbenzene with iron oxide catalyst containing K and Cr as promoters gave p-isobutylstyrene with 83% selectivity and 31% conversion. Standard conversion procedures of p-isobutylstyrene were applied to give the desired compds. I-III.</p>				
<p>IT 15687-27-1P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)</p>				
<p>RN 15687-27-1 CAPLUS</p>				
<p>CN Benzeneacetic acid, α-methyl-4-(2-methylpropyl)- (CA INDEX NAME)</p>				



L8 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:611548 CAPLUS
 DOCUMENT NUMBER: 113:211548
 ORIGINAL REFERENCE NO.: 113:35735a,35738a
 TITLE: Preparation of p-isobutylstyrene as an ibuprofen intermediate
 INVENTOR(S): Shimizu, Isao; Matsumura, Yasuo; Tokumoto, Yuichi; Uchida, Kazumichi
 PATENT ASSIGNEE(S): Nippon Petrochemicals Co., Ltd., Japan
 SOURCE: Eur. Pat. Appl., 19 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 373362	A1	19900620	EP 1989-120734	19891108 <--
EP 373362	B1	19930203		
R: CH, DE, FR, GB, IT, LI, SE				
JP 02256627	A	19901017	JP 1989-149125	19890612 <--
JP 2756828	B2	19980525		
JP 02256629	A	19901017	JP 1989-149126	19890612 <--
JP 2756829	B2	19980525		
CA 2002243	A1	19900613	CA 1989-2002243	19891106 <--
CA 2002243	C	19971230		
US 5436402	A	19950725	US 1994-323600	19941017 <--
PRIORITY APPLN. INFO.:			JP 1988-314153	A 19881213
			US 1989-435776	B1 19891113
			US 1992-917799	B1 19920720
			US 1993-62703	B1 19930514

AB Claimed is a method for preparing pure p-isobutylstyrene. The said method comprises reacting o- and/or m-isobutylethylbenzene, optionally, together with isobutylbenzene in the presence of an acid catalyst at a reaction temperature of -10 to 600° so that the production of sec-butylethylbenzene (I) does not exceed 20% by weight. Dehydrogenation of the resulting mixture of p-isobutylethylbenzene and I in the presence of a dehydrogenation catalyst containing at least one metal from groups Ib, IIb, VIa, VIIa, and VIII of the periodic table gives p-isobutylstyrene. A mixture containing isobutylbenzene (II) 81.8, o-isobutylethylbenzene (III) 7.5, m-isobutylethylbenzene (IV) 5.5, p-isobutylethylbenzene (V) 1.2 weight % was treated with CF₃SO₃H at 110° for 24 h to give II 78.7, III 3.1, IV 7.3, and V 4.7 weight %.
 Dehydrogenation of V gave p-isobutylstyrene.
 IT 15687-27-1P, α -(4-Isobutylphenyl)propionic acid
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, method for)
 RN 15687-27-1 CAPLUS
 CN Benzeneacetic acid, α -methyl-4-(2-methylpropyl)- (CA INDEX NAME)

10/923,271

